3-Methyl-1-phenyl-1H-pyrazol-5-amine

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 119 °C

Global applicability domain: Inside

Local applicability domain index: 4.25e-01

Confidence level: 6.63e-01

Nearest Neighbors from the Training Set

Image not found
3-Methyl-1-phenyl-1H-pyrazol-5-amine
Measured: 116
Predicted: 119

Image not found
Pyridine-3,4-dicarbonitrile
Measured: 80.0
Predicted: 123

Image not found
1,2,3-Benzotriazole
Measured: 100
Predicted: 124

Image not found
Kyanmethin
Measured: 183
Predicted: 172

Image not found
2-Amino-4,6-dihydroxypyrimidine
Measured: 152
Predicted: 160